

Dodecanamide, N-pentyl-

Inchi: InChI=1S/C17H35NO/c1-3-5-7-8-9-10-11-12-13-15-17(19)18-16-14-6-4-2/h3-16H2,1-2H3
InchiKey: YOWVGBBAXIJCDK-UHFFFAOYSA-N
Formula: C17H35NO
SMILES: CCCCCCCCCCCC(O)=NCCCCC
Mol. weight [g/mol]: 269.47

Physical Properties

Property code	Value	Unit	Source
hf	-474.01	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	6.054		Crippen Method
mcvol	261.940	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	757.10	K	Joback Method
tc	933.93	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407567&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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